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14. ABSTRACT
The number of particles simulated within a kinetic simulation has a direct impact on the accuracy of the results. In the case of chain-branching reactions such as those found in ionization and combustion events, the exponential growth of computational particle populations may also result in computationally intractable problems. Adaptive control of the number of computational particles is therefore an important topic for improving these types of simulations. Particle merging and its inverse splitting procedures can potentially enable this type of control, but only if they do not result in additional accumulated error. Merging multiple particles down to a single particle can be shown to either violate conservation of momentum or kinetic energy because a single particle consists of too few degrees of freedom to fully represent the original two. This has resulted in a proliferation of merging strategies relying on nearby particle pairs in velocity space or merging moments to computational grids as shown for example in Refs. [1-3]. If instead multiple particles are merged down to two rather than one, it can be shown that mass, momentum, and kinetic energy as well as center of mass and mean square deviation of position can be conserved simultaneously[4]. However, when previously attempted in this reference for electromagnetic particle-in-cell (PIC), the approach was found to result in excessive thermalization, incorrect collisionless shock wave-speeds, and was not obviously amenable to near-neighbor particle selection. To mitigate the thermalization effects, the ternary merge has been coupled with octree velocity space binning[5]. This method has been shown to match direct unmerged solutions well for several 3D3V simulations with predominately one-dimensional variations[5,6] aligned to the original coordinate system. Though these results were encouraging, the preferential selection of original spatial coordinate system for the moment decomposition suggested an orientation bias within the merge procedure. In this talk, we explore the impact of this orientation bias and several potential strategies to mitigate or eliminate it. In the process, we examine the impact of mixed second-order moments which leads to development of a merge strategy that conserves all six independent second moments using four particles. The addition of full 2nd-order spatial moment conservation can also conserve electrostatic energy for electrostatic PIC simulations to higher order in cell size for smooth electric fields. It is also shown that conserving the 0th-, 1st-, and full 2nd-moments simultaneously is in general impossible with only three particles as previously postulated in Ref. [5] except in degenerate cases. We also briefly consider the impact of dispersion between kinetic and potential energy for a sensitive 3D example case.

15. SUBJECT TERMS

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MULTIDIMENSIONAL EFFECTS ON CONSERVATIVE PARTICLE MERGING

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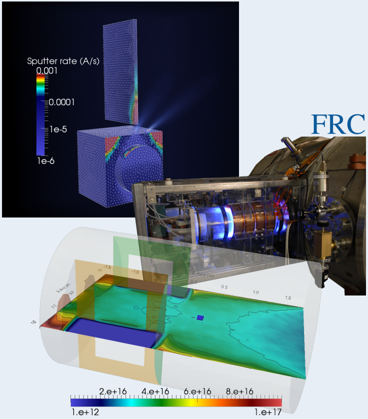
DSMC13,
Santa Fe, NM,
October 21, 2013

Outline

Spacecraft Propulsion Relevant Plasma:

- From hall thrusters to plumes and fluxes on components
- Complex reaction physics i.e. Discharge and Breakdown in FRC
- Relevant Densities often Span 6+ Orders of Magnitude
- Spatial scales of interest span μm-100m range

Electric Propulsion Plumes



Chamber Environment

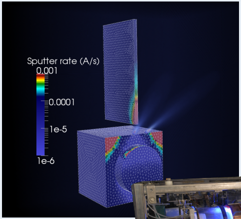
Spacecraft Propulsion Relevant Plasma:

- From hall thrusters to plumes and fluxes on components
- Complex reaction physics i.e. Discharge and Breakdown in FRC
- Relevant Densities often Span 6+ Orders of Magnitude
- Spatial scales of interest span μm-100m range

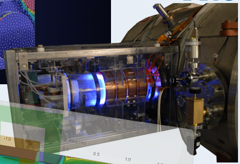
Solution?

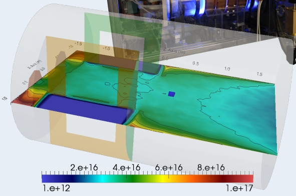
Multi-Scale and Multi-Physics Adaptive Algorithms

Electric Propulsion Plumes



FRC





Chamber Environment

Numerous Previous Merge Methods:

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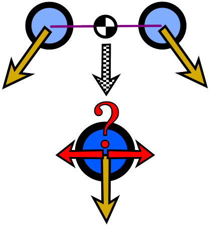
- 2:1 - Cannot Conserve Energy
  (Lapenta & Brackbill, JCP 1994)



$$w_m = \sum w_i$$
$$\vec{v}_m = \sum w_i \vec{v}_i / w_m$$

$$w_m v_m^2 < \sum w_i v_i^2 \;\; !!!$$

Prior Merging Techniques

Numerous Previous Merge Methods:

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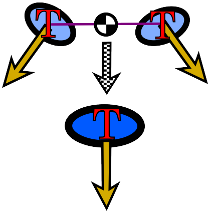
- Complex Macro-particles with Internal Energy
  (Hewett, JCP 2003)



$$w_m = \sum w_i, \quad \vec{v}_m = \sum w_i \vec{v}_i / w_m$$

$$T_m^{(int)} = \left(\sum w_i T_i^{(int)} + \sum w_i v_i^2 - w_m v_m^2 \right) / w_m$$

$$w_m \left(v_m^2 + T_m^{(int)} \right) = \sum \left(w_i v_i^2 + w_i T_i^{(int)} \right) \checkmark$$

Particle Push with $T^{(int)}$?...
Split if $(T^{(int)})^{1/2} \gg v_m$?...
In What Coord-System?...

Numerous Previous Merge Methods:

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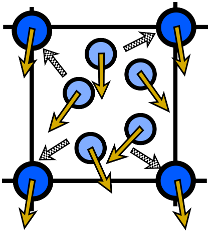
- Complex Macro-particles with Internal Energy
  (Hewett, JCP 2003)
- Merge to Grid
  (Assous et al., JCP 2003, Welch et al., JCP 2007)



Conserve Arbitrary Moments to Grid

Not Explicitly Conserved Lost?
Entropy Generation?
Shape Functions?
Grid Dependence?

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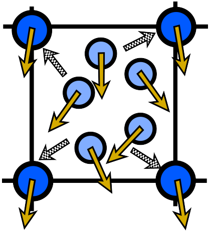
All Introduce Significant Error and/or Complexity



Conserve Arbitrary Moments to Grid

Not Explicitly Conserved Lost?
Entropy Generation?
Shape Functions?
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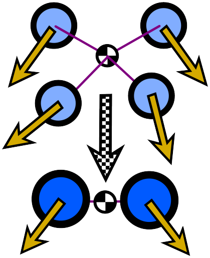
Merge to Pair $\rightarrow$ DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

(AFOSR Review 2006)



$$w_m = \sum_i^{(n+2)} w_i$$
$$\vec{\bar{v}} = \left(\sum_i^{(n+2)} w_i \vec{v}_i\right) / w_m$$
$$\overline{V^2} = \left(\sum_i^{(n+2)} w_i \left(\vec{v}_i - \vec{\bar{v}}\right)^2\right) / w_m$$

$$w_{(a/b)} = w_m/2$$
$$\vec{v}_{(a/b)} = \vec{\bar{v}} \pm \hat{\mathcal{R}}\sqrt{\overline{V^2}}$$
$$\left(\text{Similarly: } \vec{x}_{(a/b)} = \vec{\bar{x}} \pm \hat{\mathcal{R}}\sqrt{\overline{X^2}}\right)$$

Conservative Merge

Merge to Pair → DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
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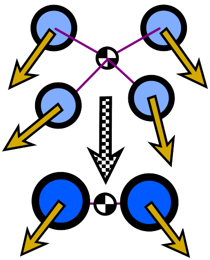
(AFOSR Review 2006)

Selection of Near Neighbors in VDF Limits Thermalization

($\approx$ Near Neighbor Pairs in 2:1 Merges that Limit Numerical Cooling)



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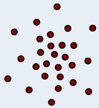
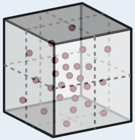
Phase-Space Decomposition

- Given a Set of Particles...



Phase-Space Decomposition

- Given a Set of Particles...
- Particles Binned in Octants



Phase-Space Decomposition

- Given a Set of Particles...
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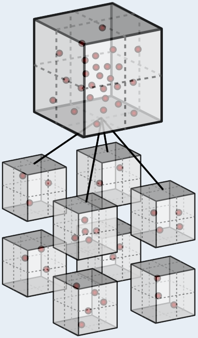

Phase-Space Decomposition

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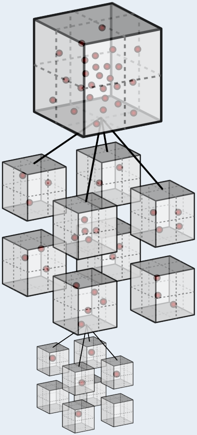

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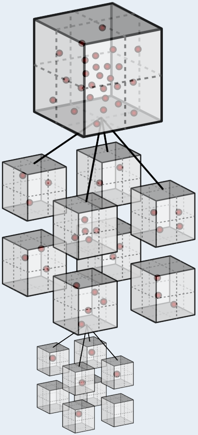
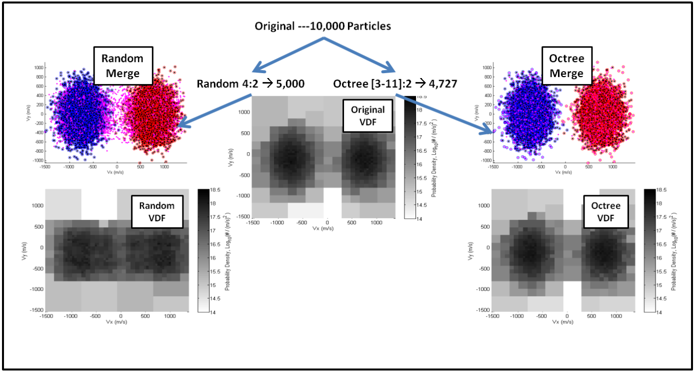
Restricts Phase-Space Diffusion to Within Local Bins



Comparison of Random vs. Octree Merge Partner Selection
(Note: Mass, Momentum, and Kinetic Energy Both Exactly Conserved)



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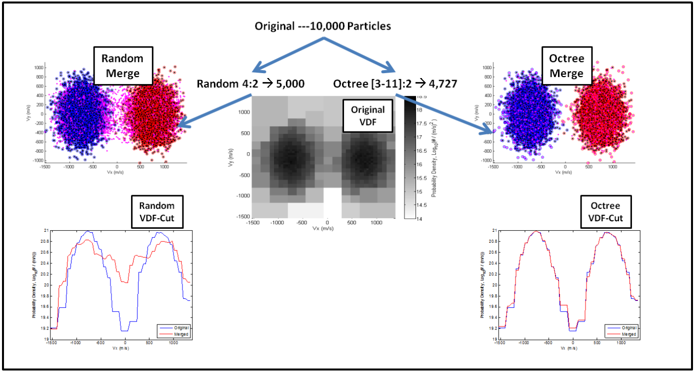
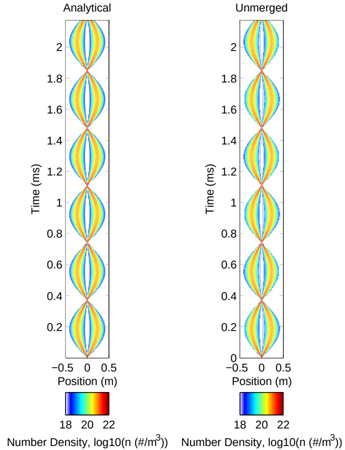


Collisionless Particles in Well

- 6000 Unmerged Particles
- Reproduces 3-4 Orders of Magnitude



Collisionless Particles in Well

- 6000 Unmerged Particles
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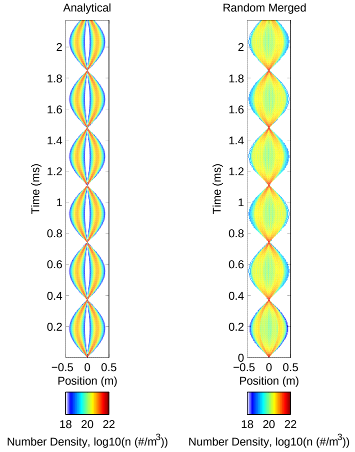
- Random Merge -> Thermalization
- 3000 First Point, 1500 First Cross
- Bi-Maxwellian Specifically Difficult



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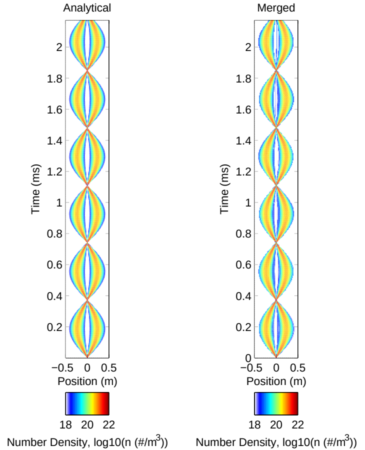

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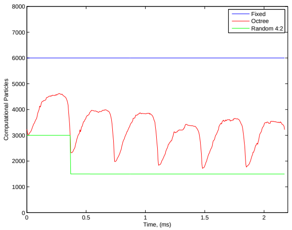

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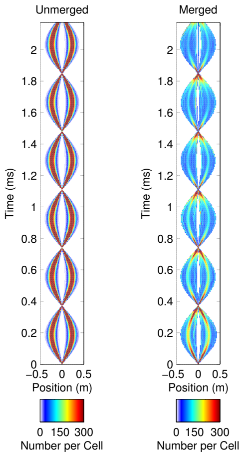
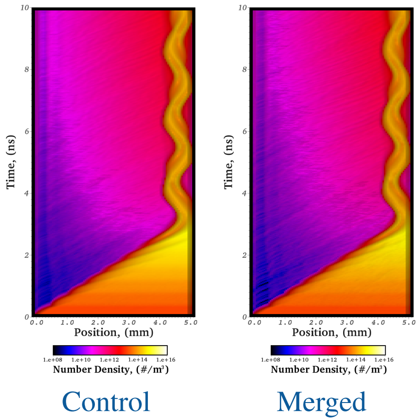
- Merge & Split Adapts Particle Count
- Computational Particles per Cell Vastly Different



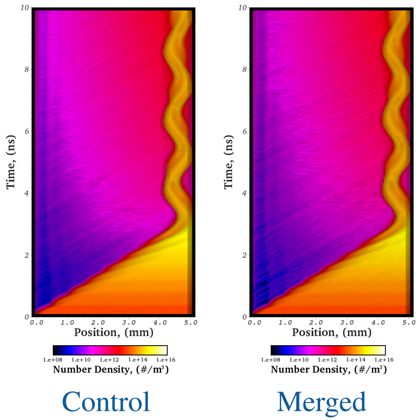
DC-Diode Test Case:

- Full 3D Electrostatic-PIC
- Averaged to 1D XT-Plot



DC-Diode Test Case:

- Full 3D Electrostatic-PIC
- Averaged to 1D XT-Plot
- 250V Cathode → Anode
- MCC-Ionization Collisions
- Secondary Emission at Cathode



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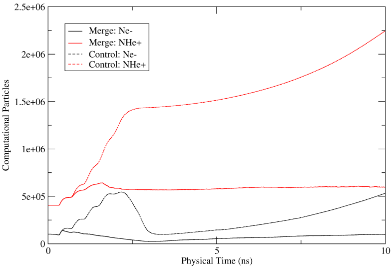
- Chain-Branching Needs Merge



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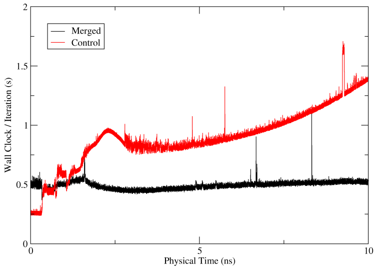
- Chain-Branching Needs Merge
- Merge Overhead Rapidly Negligible



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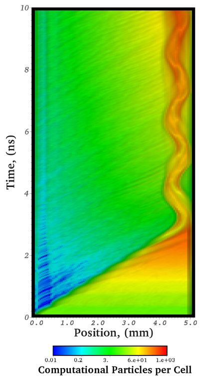
- Control: Parts/Cell $\propto$ Density



Control

Merged

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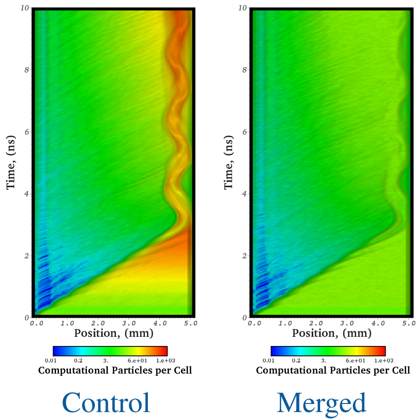
- Control: Parts/Cell ∝ Density
- Merge: Parts/Cell Much Reduced



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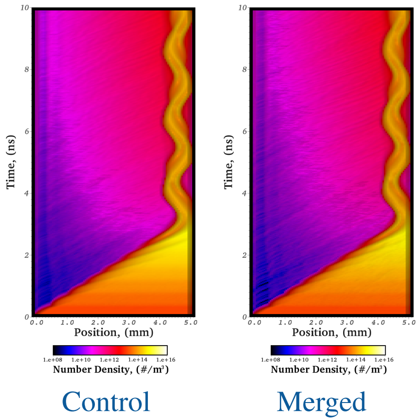
- Control: Parts/Cell $\propto$ Density
- Merge: Parts/Cell Much Reduced
- Despite Identical Densities



Multidimensional Concerns

- Conserving $[v_x^2, v_y^2, v_z^2] \rightarrow$ Axis Aligned Preference?
- 3D Well: $\Phi \propto (x^2 + y^2 + z^2)$

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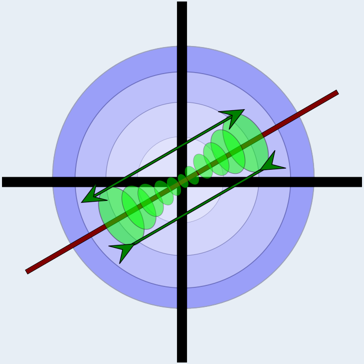

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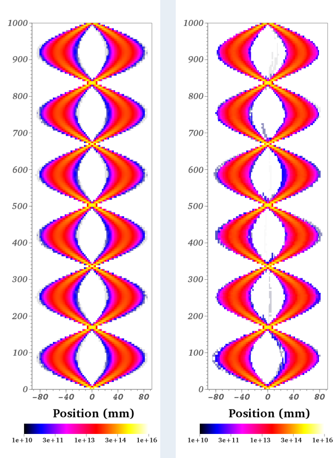
- Slice Results like 1D Well



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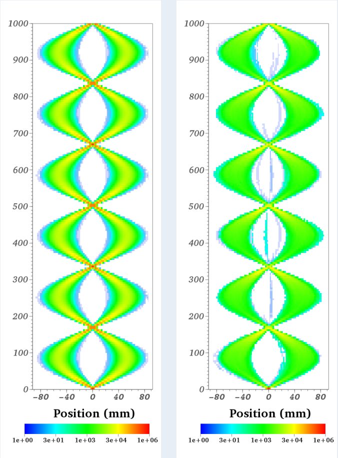

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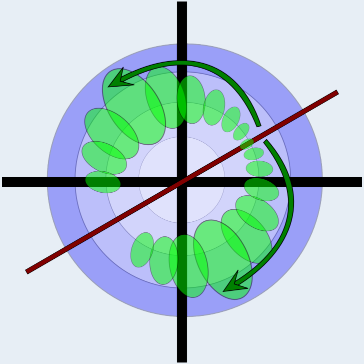
- Slice Results like 1D Well
- Next: Offset Case more Challenging



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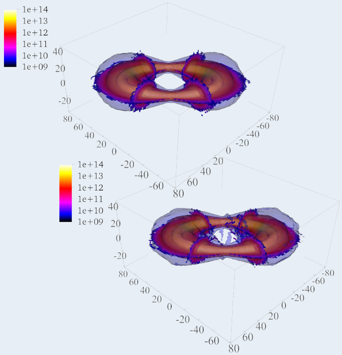
- Time Averaged Merge $\rightarrow$ Minor Scatter



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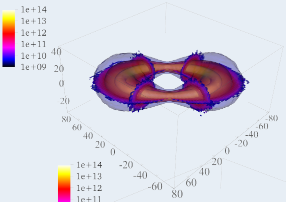
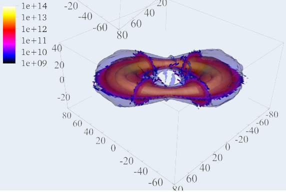
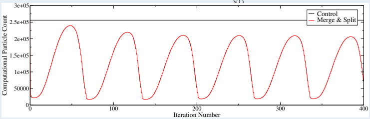
- Time Averaged Merge $\rightarrow$ Minor Scatter
- Despite Multiple Merge/Split Cycles







Parabolic Test is Insufficient

- Conserving $\mathrm{tr}(v^2)$ important due to collisional invariance
- Original Scheme also Conserved $\mathrm{tr}(x^2)$... Important?

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- Conserving tr(v^2) important due to collisional invariance
- Original Scheme also Conserved tr(x^2)... Important?
- Potential Energy Conservation via Taylor Expansion

$$\overline{\Phi} = \frac{\sum_p^k w^{(p)} \left[\Phi(\overline{x_i}) + \frac{\partial \Phi}{\partial x_i}\Big|_{\overline{x_i}} (x_i^{(p)} - \overline{x_i}) + \frac{1}{2} \frac{\partial^2 \Phi}{\partial x_i \partial x_j}\Big|_{\overline{x_i}} (x_i^{(p)} - \overline{x_i})(x_j^{(p)} - \overline{x_j}) \right]}{\sum_p^k w^{(p)}} + o\left(\Delta x^3 \Big|_{\max} \right)$$

$$= \Phi(\overline{x_i}) + \frac{\partial^2 \Phi}{\partial x_i \partial x_j}\Big|_{\overline{x_i}} \frac{\sum_p^k w^{(p)} \left[(x_i^{(p)} - \overline{x_i})(x_j^{(p)} - \overline{x_j}) \right]}{\sum_p^k w^{(p)}} + o\left(\Delta x^3 \Big|_{\max} \right)$$

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- Original Scheme also Conserved tr(x^2)... Important?
- Potential Energy Conservation via Taylor Expansion
- $O\left(\Delta x^2\big|_{\max}\right)$ Energy Conservation Requires Center of Mass, $\overline{x_i}$, Only

$$\overline{\Phi} = \frac{\sum_p^k w^{(p)}\left[\Phi(\overline{x_i}) + \frac{\partial\Phi}{\partial x_i}\Big|_{\overline{x_i}}(x_i^{(p)} - \overline{x_i}) + \frac{1}{2}\frac{\partial^2\Phi}{\partial x_i \partial x_j}\Big|_{\overline{x_i}}(x_i^{(p)} - \overline{x_i})(x_j^{(p)} - \overline{x_j})\right]}{\sum_p^k w^{(p)}} + O\left(\Delta x^3\big|_{\max}\right)$$

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- Next Order? Requires Full $(x_i^{(p)}-\overline{x_i})(x_j^{(p)}-\overline{x_j})$ Tensor for Arbitrary Φ

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Issues with Parabolic Case

Parabolic Test is Insufficient

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- Original Scheme also Conserved $\mathrm{tr}(x^2)$... Important?
- Potential Energy Conservation via Taylor Expansion
- $O\left(\Delta x^2\big|_{\max}\right)$ Energy Conservation Requires Center of Mass, $\overline{x_i}$, Only
- Next Order? Requires Full $(x_i^{(p)}-\overline{x_i})(x_j^{(p)}-\overline{x_j})$ Tensor for Arbitrary Φ
- But Parabolic Potential $\rightarrow$ Diagonal Hessian!
- $\therefore$ Accidental Exact Potential Conservation via Diagonal 2^{nd} Moment Cons.

$$\overline{\Phi} = \frac{\sum_p^k w^{(p)}\left[\Phi(\overline{x_i}) + \frac{\partial\Phi}{\partial x_i}\Big|_{\overline{x_i}}(x_i^{(p)}-\overline{x_i}) + \frac{1}{2}\frac{\partial^2\Phi}{\partial x_i\partial x_j}\Big|_{\overline{x_i}}(x_i^{(p)}-\overline{x_i})(x_j^{(p)}-\overline{x_j})\right]}{\sum_p^k w^{(p)}} + O\left(\Delta x^3\big|_{\max}\right)$$

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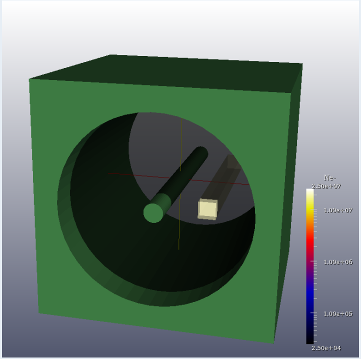
Increased Complexity First Attempt...

- Annular Potential:
  $\Phi \propto log(r/r_{\text{in}})/log(r_{\text{in}}/r_{\text{out}})$
- Non-Trivial Cartesian Derivative of Φ



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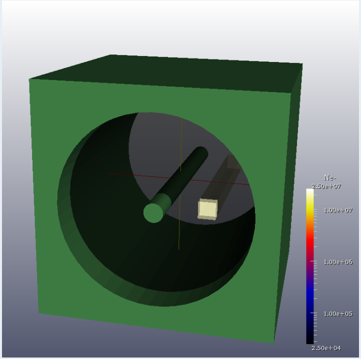
- Different Periods per Particle - Non-Periodic unlike Parabolic Well
- Part./Cell Drops & #-Cells Active Grows



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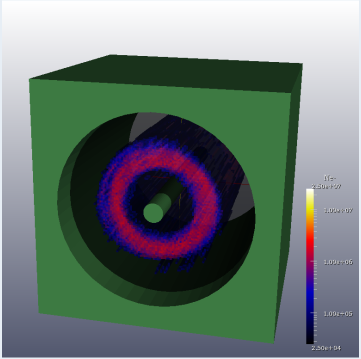
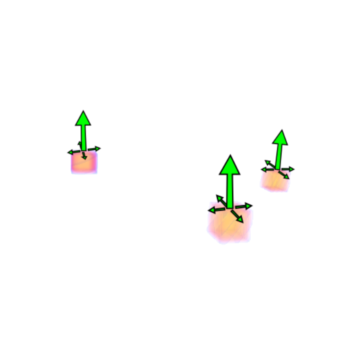
Not a Good Repeating Merge/Split Test



Increased Complexity Second Attempt...

- Spherical Potential: $\Phi \propto 1/r$

Without Merge & Split



Increased Complexity Second Attempt...

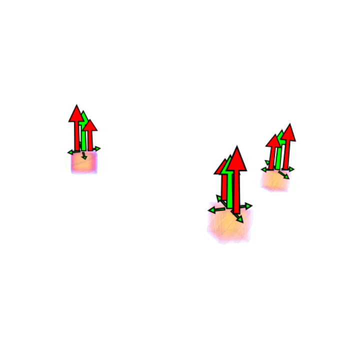
- Spherical Potential: $\Phi \propto 1/r$
- Slight $\Delta X \rightarrow$ Orbits Unsynchronized

Without Merge & Split

Increased Complexity Second Attempt...

- Spherical Potential: $\Phi \propto 1/r$
- Slight $\Delta X \rightarrow$ Orbits Unsynchronized
- Periods Synched via Orbital Mech. Eqns.

Without Merge & Split



Increased Complexity Second Attempt...

- Spherical Potential: $\Phi \propto 1/r$
- Slight $\Delta X \rightarrow$ Orbits Unsynchronized
- Periods Synched via Orbital Mech. Eqns.
- Periodic with Full Nonlinear-C.N. Push

Without Merge & Split

Increased Complexity Second Attempt...

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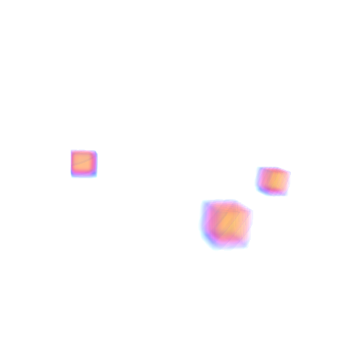
- Slight $\Delta X \rightarrow$ Orbits Unsynchronized
- Periods Synched via Orbital Mech. Eqns.
- Periodic with Full Nonlinear-C.N. Push
- Adding Merge & Split:
  Energy Conservation OK
  Accuracy: Scatter + Dispersion?

Including Merge & Split



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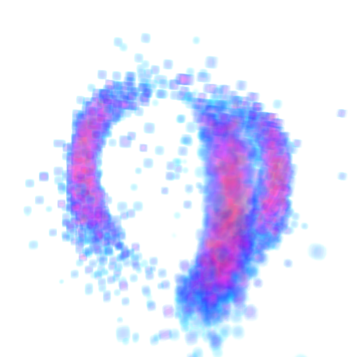
Source of Dispersion?

Including Merge & Split



$O(\Delta x^3_{\text{cell}})$ Potential Conservation:

- Remap must Preserve Identical Contraction, $\partial_i \partial_j \Phi : \overline{\Delta x_i \Delta x_j}$

$$\begin{bmatrix} \Phi_{xx} & \Phi_{xy} & \Phi_{xz} \\ \Phi_{yx} & \Phi_{yy} & \Phi_{yz} \\ \Phi_{zx} & \Phi_{zy} & \Phi_{zz} \end{bmatrix} : \begin{bmatrix} \overline{\Delta x \Delta x} & \overline{\Delta x \Delta y} & \overline{\Delta x \Delta z} \\ \overline{\Delta y \Delta x} & \overline{\Delta y \Delta y} & \overline{\Delta y \Delta z} \\ \overline{\Delta z \Delta x} & \overline{\Delta z \Delta y} & \overline{\Delta z \Delta z} \end{bmatrix}$$

$O(\Delta x^3_{\text{cell}})$ Potential Conservation:

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- 2-Particle Only Reproduces Diagonal with $x_i^{(a/b)} = \overline{x_i} \pm \epsilon_i$ if $\epsilon_i = \overline{\Delta x_i^2}^{1/2}$

$$\begin{bmatrix} \overline{\Delta x \Delta x} & \overline{\Delta x \Delta y} & \overline{\Delta x \Delta z} \\ \overline{\Delta y \Delta x} & \overline{\Delta y \Delta y} & \overline{\Delta y \Delta z} \\ \overline{\Delta z \Delta x} & \overline{\Delta z \Delta y} & \overline{\Delta z \Delta z} \end{bmatrix} \neq \begin{bmatrix} \epsilon_x \epsilon_x & \epsilon_x \epsilon_y & \epsilon_x \epsilon_z \\ \epsilon_y \epsilon_x & \epsilon_y \epsilon_y & \epsilon_y \epsilon_z \\ \epsilon_z \epsilon_x & \epsilon_z \epsilon_y & \epsilon_z \epsilon_z \end{bmatrix}$$

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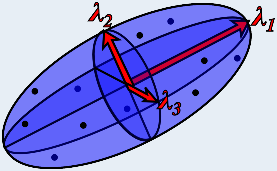
$$\begin{bmatrix} \overline{\Delta x \Delta x} & \overline{\Delta x \Delta y} & \overline{\Delta x \Delta z} \\ \overline{\Delta y \Delta x} & \overline{\Delta y \Delta y} & \overline{\Delta y \Delta z} \\ \overline{\Delta z \Delta x} & \overline{\Delta z \Delta y} & \overline{\Delta z \Delta z} \end{bmatrix} =$$



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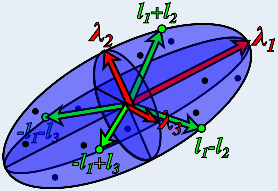
(3-Particles = Plane & $\lambda_3 = 0$; 2-Particles = Line & $\lambda_2, \lambda_3 = 0$)

$$\begin{bmatrix} \overline{\Delta x \Delta x} & \overline{\Delta x \Delta y} & \overline{\Delta x \Delta z} \\ \overline{\Delta y \Delta x} & \overline{\Delta y \Delta y} & \overline{\Delta y \Delta z} \\ \overline{\Delta z \Delta x} & \overline{\Delta z \Delta y} & \overline{\Delta z \Delta z} \end{bmatrix} =$$



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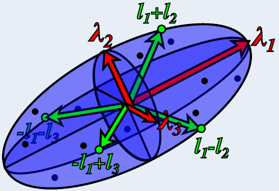
- Same $\rightarrow$ 4 Merge for 2nd-Vel. Moment
- "Principal Component Analysis"

$$\begin{bmatrix} \overline{\Delta x \Delta x} & \overline{\Delta x \Delta y} & \overline{\Delta x \Delta z} \\ \overline{\Delta y \Delta x} & \overline{\Delta y \Delta y} & \overline{\Delta y \Delta z} \\ \overline{\Delta z \Delta x} & \overline{\Delta z \Delta y} & \overline{\Delta z \Delta z} \end{bmatrix} =$$



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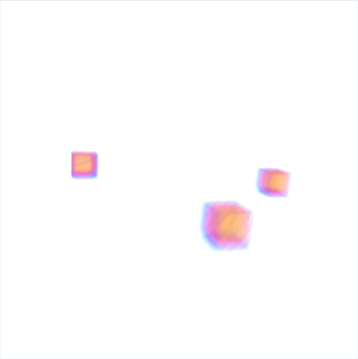
- Same $\rightarrow$ 4 Merge for 2^{nd}-Vel. Moment
- "Principal Component Analysis"
- Improved but Non-Negligible Scatter and Dispersion



Kinetic Potential Energy Scatter:

- A Closer look at Merge $\to$ 2
- $\approx$ Match $Sgn\left(\epsilon_i^{(v)}\right)$ to $Sgn(\Delta v_i \Delta v_j)$ Moments
- Select $Sgn\left(\epsilon_i^{(x)}\right)$ to Match $Sgn(\Delta x_i \Delta v_i)$

$$\begin{bmatrix} - & Sgn\left(\epsilon_x^{(v)}\epsilon_y^{(v)}\right) & Sgn\left(\epsilon_x^{(v)}\epsilon_z^{(v)}\right) \\ Sgn\left(\epsilon_y^{(v)}\epsilon_x^{(v)}\right) & - & Sgn\left(\epsilon_y^{(v)}\epsilon_z^{(v)}\right) \\ Sgn\left(\epsilon_z^{(v)}\epsilon_x^{(v)}\right) & Sgn\left(\epsilon_z^{(v)}\epsilon_y^{(v)}\right) & - \end{bmatrix} \approx$$

$$\begin{bmatrix} - & Sgn\left(\overline{\Delta v_x \Delta v_y}\right) & Sgn\left(\overline{\Delta v_x \Delta v_z}\right) \\ Sgn\left(\overline{\Delta v_y \Delta v_x}\right) & - & Sgn\left(\overline{\Delta v_y \Delta v_z}\right) \\ Sgn\left(\overline{\Delta v_z \Delta v_x}\right) & Sgn\left(\overline{\Delta v_z \Delta v_y}\right) & - \end{bmatrix}$$

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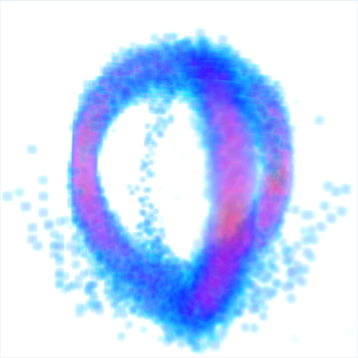
- Why Stop at just *XV* Sign?

$$\epsilon_i^{(x)} = \left(\overline{\Delta x_i \Delta v_i}\right) / \epsilon_i^{(v)}$$



DISPERSION FROM *XV* SCATTER?

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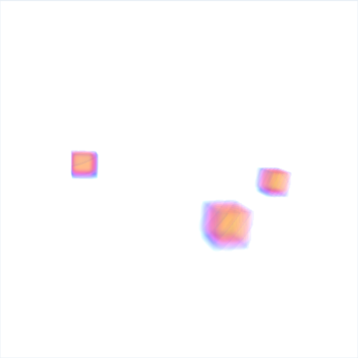
  $$\epsilon_i^{(x)} = \left(\overline{\Delta x_i \Delta v_i}\right) / \epsilon_i^{(v)}$$
- Much Improved Scatter & Dispersion



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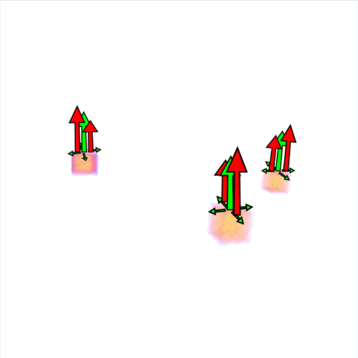
- Sphere Sensitive: Kinetic <-> Potential



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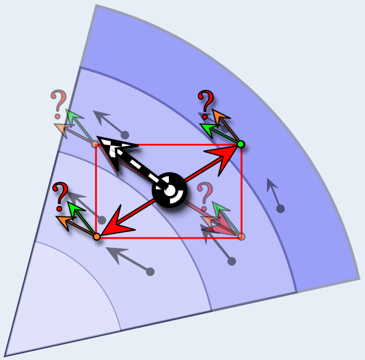
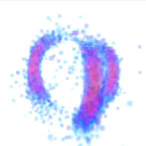
  $$\epsilon_i^{(x)} = \left(\overline{\Delta x_i \Delta v_i}\right) / \epsilon_i^{(v)}$$
- Much Improved Scatter & Dispersion
- Sphere Sensitive: Kinetic <-> Potential
- K.E. & P.E. Conserved Independently...
  XV-Moment $\rightarrow$ Better Combination



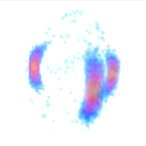
Review Sphere Test Results

Merge Results after 1-Cycle

No Merge

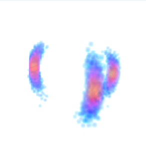


Random Sign



PCA

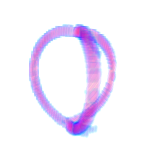
XV-Sign



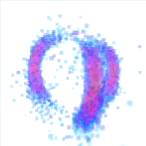
XV-Full

Note: Results Due to Extreme Case Sensitivity
C.N. Push Required for Stability
Period Sync Required for Initial Conditions

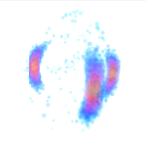
Merge Results after 1-Cycle



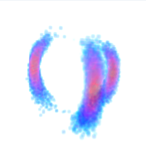
Not Synched



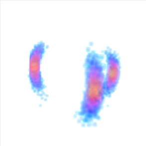
Random Sign



PCA



XV-Sign

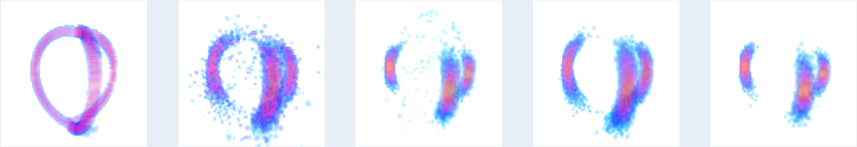


XV-Full

Note: Results Due to Extreme Case Sensitivity
C.N. Push Required for Stability
Period Sync Required for Initial Conditions

Review Sphere Test Results

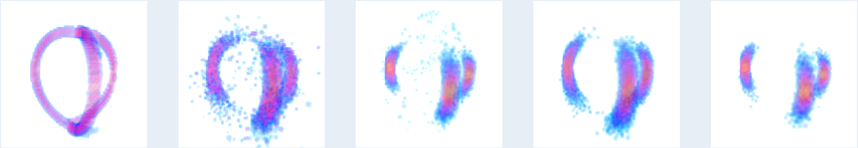
Merge Results after 1-Cycle



Not Synched | Random Sign | PCA | *XV*-Sign | *XV*-Full

Note: Results Due to Extreme Case Sensitivity
C.N. Push Required for Stability
Period Sync Required for Initial Conditions
Result of Minor Velocity Difference Across IC Box

Merge Results after 1-Cycle

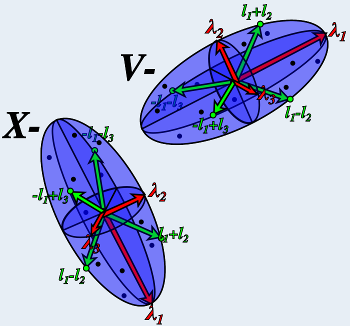


Not Synched | Random Sign | PCA | *XV*-Sign | *XV*-Full

Note: Results Due to Extreme Case Sensitivity
C.N. Push Required for Stability
Period Sync Required for Initial Conditions
Result of Minor Velocity Difference Across IC Box
Merge Scatter in Cells $<$ Synch ΔV

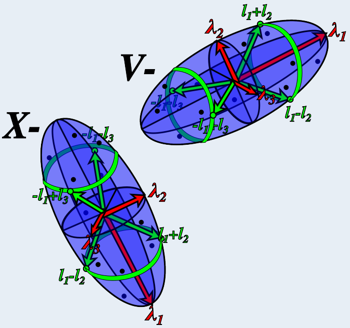
PCA + *XV*-Merge?

- Both Partially Inhibited Dispersion



PCA + *XV*-Merge?

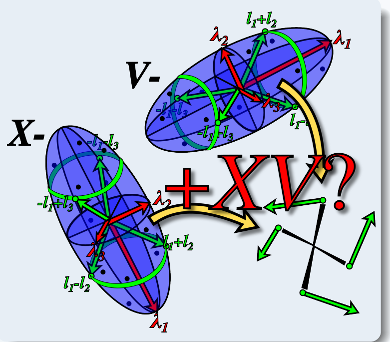
- Both Partially Inhibited Dispersion
- Extra Degrees of Freedom in PCA



Future Work: Combined PCA/*XV* Merge

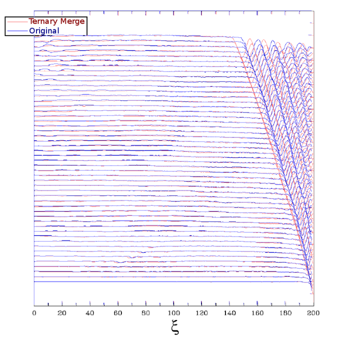
PCA + *XV*-Merge?

- Both Partially Inhibited Dispersion
- Extra Degrees of Freedom in PCA
- Use Extra DOF for XV-Match?



PCA + *XV*-Merge?

- Both Partially Inhibited Dispersion
- Extra Degrees of Freedom in PCA
- Use Extra DOF for XV-Match?
- *XV*-Dispersion Source of Error in Lapenta's MHD Slow Shock?



Lapenta - JCP 181, 317-337 (2002)

Integrate R&D w/ Production TODO:

- Combine PCA and *XV* Merges

  (Martin/Lederman)

- Remap <-> Vlasov <-> Fluid

  (Martin/Bilyeu/TBD)

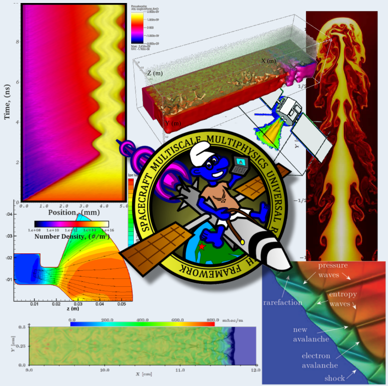
- Implicit/Multiscale GPU-Accel. PIC

  (Lederman/Gimelsheins/Martin/TBD)

- GPU Accelerated Chemical Kinetics / CR Ar-Ne-Xe-Molecular Models

  (Le/Cole*/Kapper* PhD Research)

*Note: Former Co-op Student Work to be Integrated into Framework



Thank You

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(PM: Dr. J. Luginsland)

Questions?